CHARGED PARTICLES

IN

ELECTROSTATIC AND ELECTROMAGNETIC FIELDS

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CHARGED PARTICLES IN ELECTROSTATIC AND ELECTROMAGNETIC FIELDS

by

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CHARGED PARTICLES IN ELECTROSTATIC AND ELECTROMAGNETIC FIELDS

Introduction

One of the most complex problems of Modern Physics is the formulation of a theory which will account in entirety for the many phenomena which arise from the interaction between charged particles and radiation fields. The first man to attack this problem with any apparent success was H. A. Lorentz, when he developed a classical theory of the electron using the highly investigated Maxwell's equations. He assumed that the electron had a finite dimension, specifically, a radius R and that there existed internally a finite density of electricity d^*. With this as a foundation he wrote the following equations to express the relation between the electron and the electromagnetic fields.

$$\text{Div } \bar{H} = 0 \qquad \text{Curl } \bar{H} = \frac{1}{c}\left(\frac{\partial \bar{E}}{\partial t} + d^*\bar{V}\right) \tag{1.1}$$

$$\text{Div } \bar{E} = d^* \qquad \text{Curl } \bar{E} = -\frac{1}{c}\frac{\partial \bar{H}}{\partial t}$$

where $\bar{V}$ is the velocity of the electricity at the point where the microscopic density is d^*, where $\bar{E}$ and $\bar{H}$ are the electric and magnetic vectors respectively of the incident field. To these equations we have to add the one expressing the mechanical force exerted on a unit charge by an electromagnetic field. The approximate result is

$$\bar{F} = m\frac{d\bar{V}}{dt} - \frac{2}{3}\left(\frac{e^2}{c^3}\right)\left(\frac{d^2\bar{V}}{dt^2}\right) = e[\bar{E} + (\bar{V}/c) \times \bar{H}] \tag{1.2}$$

He was able to compute the radiation reaction term which involved the second derivative of the velocity by assuming the radius of the electron as small and then expanding this force in terms of a power series of the radius,

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$$\bar{F} = m\frac{d\bar{V}}{dt} - \frac{2}{3}\left(\frac{e_0}{c^3}\right)\left(\frac{d^2\bar{V}}{dt^2}\right) = e[\bar{E} + (\bar{V}/c) \times \bar{H}] \qquad 1.2$$

He was able to compute the radiation reaction term which involved the second derivative of the velocity by assuming the radius of the electron as small and then expanding this force in terms of a power series of the radius,

using only the zeroth term.

Under analysis these equations showed inconsistencies, one of the most serious defects being that they failed to explain the very existence of particles. Another serious difficulty was that they failed to explain the so called stationary states in which the electron could exist without the radiation of energy. By Lorentz's method the electron would be continually giving up energy and would promptly spiral into the nucleus.

His equations did not hold from the relativity standpoint, because size was not a relativistically invariant concept and a sphere in one frame of reference would not be a sphere in another frame of reference. Because of this it was found advisable to discontinue the idea of an electron of finite radius and consider one as concentrated at a point or a point electron. The main difficulty with this theory was that the electron had to have an infinite self energy. It was hoped that this would be overcome when extended to the Quantum Theory, however, it showed itself in divergence integrals when one tried to solve the Wave Equation. C. J. Eliezer, in a recent paper, offered a partial solution to the problem by using some of Dirac's refinements. The infinities existing in the Classical Theory were subtracted in a Lorentz invariant way. These classical results were then taken over into the Quantum Theory. The Hamiltonian Equations of motion were expressed in terms of a "λ limiting process", introduced by Wentzel, whereby λ was a small time like vector which allowed exact equations only with the limit of λ tending to zero. This process was found to be most successful when divergences were eliminated from the radiation theory.

It is the purpose of this paper to examine attempts of a solution of

the above mentioned problem, carrying through as a foundation solutions of the non-relativistic Schrödinger equation and the relativistic Dirac equation of an electron in a central electrostatic field. This approach is chosen because with the electrostatic field we are able to effect solutions with a minimum of trouble due to the potential being expressed only as a scalar quantity. When carried over to the electromagnetic field the potential is first expressed as a vector and a scalar for the non-relativistic approach and as a four-vector for the solution of the relativistic Dirac equation.

If these solutions are applied to observed physical phenomena, then we find that they are a close approximation to the motion of Hydrogen-like atoms where if we use the Schrödinger approach we have a spin-less electron which needs the Pauli spin; however, use of Dirac's principles mathematically includes this spin.

A. Electrostatic Fields

Building a Hamiltonian

In the case of the Hydrogen Atom where we have a positively charged mucleus with a charge +Ze acting on an electron -e , we may express the Coulomb interaction between the two with a potential function

$$V(r) = -Ze^2/r. \qquad 2.1$$

Calculated values of the energy levels should correspond to the observed, if relativity effects are disregarded, with a completed solution of the time independent equation.

$$H_o\psi_o = E_o\psi_o \qquad 2.2$$

where ψ_o is the wave function; E_o is the energy eigenvalue, and H_o is the Hamiltonian. To construct this Hamiltonian we have to become familiar with some of the elementary principles of Analytical Mechanics. One of the laws of Classical Mechanics states that when a system is subject to conservative forces then we may use the differential equations in the Lagragian form

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{X}_i}\right) - \frac{\partial L}{\partial X_i} = 0 \qquad (i = 1,2, \ldots . n) \qquad 2.3$$

$$L = T - V$$

where T is the Kinetic and V the potential Energy. (2.3) are the Euler-Lagrange Equations of a variational problem.

The momenta are defined as

$$p_i = \frac{\partial L}{\partial \dot{X}_i} \qquad 2.4$$

The n differential equations (2.3) of the second order may be changed to 2n differential equations of the first order as follows:

Perform an integration on (2.4) so

$$\int \partial L = p_i \int \partial \dot{X}_i$$

$$L = p_i \dot{X}_i + \text{constant},$$

or in a more common form we have the Hamiltonian function.

$$H_o = p_i \dot{X}_i - L \qquad 2.5$$

The Kinetic Energy can be represented as $T = 1/2\ m_i \dot{X}_i^2$ or

$$2T = m_i \dot{X}_i^2 = p_i \dot{X}_i \qquad 2.6$$

Putting this in (2.5)

$$H_o = 2T - L = 2T - T + V$$

$$\therefore H_o = T + V \qquad 2.7$$

The Hamiltonian H is considered a constant of motion which is equal to the sum of the potential and kinetic energies.

If T is expressed in terms of its momentum operator

$$H_o = \frac{1}{2m_i} (m_i v_i)^2 + V$$

and

$$H_o = \frac{p_i^2}{2m_i} + V \qquad 2.8$$

The substitution of the quantum operator

$$p_i = + \frac{h}{2\pi i} \frac{\partial}{\partial X_i}$$

into (2.8) gives

$$H_o = - \frac{h^2}{8\pi^2 m_i} \frac{\partial^2}{\partial X_i^2} + V \qquad 2.9$$

This general Hamiltonian may be used as the Hamiltonian of (2.2) if certain designations are made.

The mass m_i may be considered the reduced mass M

$$M = \frac{M_e M_p}{M_e + M_p}$$

where M_e is the mass of the electron and M_p the mass of the proton. If we allow no motion of the nucleus we arrive at energy eigenvalues in terms of M_e. Allowing motion of the nucleus makes only a small change in the energy, namely the reduced mass M is substituted for M_e. Therefore equations will be solved assuming a fixed nucleus but using a reduced mass M to give us the correct energy values.

The coordinates X_i will be the regular cartesian coordinates X, Y and Z. Therefore the new Hamiltonian will be

$$H_o = -\frac{h^2}{8\pi^2 M}\left[\frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial Y^2} + \frac{\partial^2}{\partial Z^2}\right] + V_{(r)} \qquad 2.11$$

or

$$H_o = -\frac{h^2}{8\pi^2 M}\Delta XYZ + V_{(r)} \qquad 2.12$$

where Δ is the Laplacian.

Separation of Schrödinger Equation

By placing (2.12) into (2.2) we have the following equation called the time independent Schrödinger equation.

$$\Delta\psi + \frac{8\pi^2 M}{h^2}[E - V(r)]\psi = 0 \qquad 3.1$$

The best method to solve this equation is to express the ψ's in terms of polars.

$$\therefore \psi = \psi(r, \theta, \phi)$$

and since

$$\Delta\psi(X,Y,Z) = \frac{\partial^2\psi}{\partial X^2} + \frac{\partial^2\psi}{\partial Y^2} + \frac{\partial^2\psi}{\partial Z^2}$$

$$M = \frac{M_e M_p}{M_e + M_p}$$

where M_e is the mass of the electron and M_p the mass of the proton. If we allow no motion of the nucleus we arrive at energy eigenvalues in terms of M_e. Allowing motion of the nucleus makes only a small change in the energy, namely the reduced mass M is substituted for M_e. Therefore equations will be solved assuming a fixed nucleus but using a reduced mass M to give us the correct energy values.

The coordinates X_i^1 will be the regular cartesian coordinates X, Y and Z. Therefore the new Hamiltonian will be

$$H^o = -\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial Y^2} + \frac{\partial^2}{\partial Z^2}\right) + V(r) \qquad 2.11$$

or

$$H^o = -\frac{\hbar^2}{2M}\Delta XYZ + V(r) \qquad 2.12$$

where Δ is the Laplacian.

Separation of Schrödinger Equation

By placing (2.12) into (2.5) we have the following equation called the time independent Schrödinger equation.

$$\Delta\psi + \frac{2M}{\hbar^2}[E - V(r)]\psi = 0 \qquad 3.1$$

The best method to solve this equation is to express the ψ in terms of polars.

$$\therefore \psi = \psi(r, \theta, \phi)$$

and since

$$\Delta\psi(X,Y,Z) = \frac{\partial^2\psi}{\partial X^2} + \frac{\partial^2\psi}{\partial Y^2} + \frac{\partial^2\psi}{\partial Z^2}$$

then

$$\Delta\psi(r,\theta,\phi) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2} \qquad 3.2$$

By putting (3.2) into (3.1) we find that

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2} + \frac{8\pi^2M}{h^2}[E - V]\psi = 0 \qquad 3.3$$

This equation may be separated by allowing the eigenfunction to be expressed in terms of three quantities

$$\therefore\psi = R_{(r)}\,\Theta_{(\theta)}\,\Phi_{(\phi)} \qquad 3.4$$

Placing this into (3.3) where V is a function of r alone gives

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\Theta\Phi\frac{dR}{dr}\right) + \frac{1}{r^2\sin\theta}\frac{d}{d\theta}\left(\sin\theta\, R\Phi\frac{d\Theta}{d\theta}\right) + \frac{1}{r^2\sin^2\theta}R\Theta\frac{d^2\Phi}{d\phi^2}$$

$$+ \frac{8\pi^2M}{h^2}[E - V_{(r)}]R\Theta\Phi = 0$$

After multiplying by $\dfrac{r^2}{R\Theta\Phi}$ the equation becomes

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \left\{\frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \frac{1}{\sin^2\theta\,\Phi}\frac{d^2\Phi}{d\phi^2}\right\}$$

$$+ \frac{8\pi^2M}{h^2}r^2[E - V(r)] = 0 \qquad 3.5$$

Since the $\{\ \}$ part of (3.5) contains no r's we can call it a constant C and solve the rest of the equation. Solution of the $\{\ \}$ terms for a finite ψ gives us $C = j(j+1)$ where j is the azimuthal quantum number which is analogous to the quantum number K in the old theory. Also $j = m, m+1, \ldots$ where m is the axial quantum number.

From (3.5) we have the following equation

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{8\pi^2M}{h^2}r^2\left[E - V(r)\right] - j(j+1) = 0 \qquad 3.6$$

Solution of the Radial Equation

After slight rearrangement the radial equation (3.6) becomes

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{8\pi^2Mr^2}{h^2}\left[E - V - \frac{j(j+1)h^2}{8\pi^2Mr^2}\right] = 0$$

Multiply through by R and complete the differentiation so

$$r^2\frac{d^2R}{dr^2} + 2r\frac{dR}{dr} + \frac{8\pi^2Mr^2}{h^2}\left[E - V - \frac{j(j+1)h^2}{8\pi^2Mr^2}\right]R = 0 \qquad 3.7$$

As a further simplification we choose the following relation as a substitution

$$Y = rR \qquad 3.8$$

We find that this is a good choice because in the normalization of the radial function in polars we have

$$\int RR^*r^2dr = 1$$

which will become, upon substitution of (3.8),

$$\int YY^*dr = 1$$

Putting (3.8) into (3.7) brings the following results

$$\frac{d^2Y}{dr^2} + \frac{8\pi^2M}{h^2}\left[E - V(r) - \frac{j(j+1)h^2}{8M\pi^2r^2}\right]Y = 0$$

If we use the Coulomb Potential found in (2.1) and make the following substitutions $p = 2ar$ where $a^2 = -\frac{8\pi^2ME}{h^2}$

and $$B = \frac{MZe^2}{a(\frac{h^2}{4\pi^2})} = \frac{4\pi^2 MZe^2}{ah^2} \qquad 3.9$$

and then making a change of variable from r to p where p is not to be confused with the momentum operator, the resulting equation will be

$$\frac{d^2Y}{dp^2}(2a)^2 + [-a^2 + \frac{8\pi^2 MZe^2}{rh^2} - \frac{j(j+1)}{r^2}]Y = 0$$

This can be reduced further to

$$\frac{d^2Y}{dp^2} + [-\frac{1}{4} + \frac{B(2a)}{4a^2 r} - \frac{j(j+1)}{4a^2 r^2}]\ Y = 0$$

and the final form being

$$\frac{d^2Y}{dp^2} + [-\frac{1}{4} - \frac{j(j+1)}{p^2} + \frac{B}{p}]\ Y = 0 \qquad 3.10$$

where $0 \leq p \leq \infty$

This equation has improper points at the origin namely when $p = 0$ and $p = \infty$. When p is very large, that is $p \to \infty$, then (3.10) becomes

$$\frac{d^2Y}{dp^2} - \frac{1}{4}Y = 0 \qquad 3.11$$

The solutions to this equation are

$$Y = Ae^{\pm p/2}$$

The minus term is the only one that gives a well behaved solution because the plus term is improper when p goes to ∞. Thereby $Y = Ae^{-p/2}$ 3.12 is the good solution. To be perfect we should use all the terms, however we want to simplify the solution so we let p approach 0, then equation (3.10) becomes

and $$B = \frac{AE\varepsilon_s^2}{a(\frac{Ir_s^2}{4\Pi^2})} = \frac{4\Pi^2 AE\varepsilon_s^2}{ar_s^2} \qquad 3.9$$

and then making a change of variable from r to p where p is not to be confused with the momentum operator, the resulting equation will be

$$\frac{d^2Y}{dp^2}(2a)^2 + [-\varepsilon_s^2 + \frac{B^2\varepsilon_s^2 E}{\pi^2 p^2} - \frac{4(j+j)}{p^2}]Y = 0$$

This can be reduced further to

$$\frac{d^2Y}{dp^2} + [-\frac{1}{4} + \frac{E(2a)}{4a^2\pi^2} - \frac{4(j+j)}{4a^2\pi^2}]Y = 0$$

and the final form being

$$\frac{d^2Y}{dp^2} + [\frac{1}{4} - \frac{4(j+j)}{p^2} + \frac{E}{p}]Y = 0 \qquad 3.10$$

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$$\frac{d^2Y}{dp^2} - \frac{j(j+1)}{p^2} Y = 0 \qquad 3.13$$

If we try a substitution

$$Y = p^K \text{ into } (3.13)$$

then

$$K(K-1)p^{K-2} - \frac{j(j+1)p^K}{p^2} = 0$$

or

$$K(K-1)p^{K-2} - j(j+1)p^{K-2} = 0$$

so

$$K(K-1) = j(j+1)$$

or

$$K^2 - K - j(j+1) = 0$$

$$K = \frac{1 \pm \sqrt{1 + 4j(j+1)}}{2} = \frac{1 \pm \sqrt{4j^2 + 4j + 1}}{2}$$

$$K = \frac{1 \pm (2j+1)}{2}$$

so $K = j + 1$ with the +

and $K = -j$ with the -

$\therefore K = j + 1, -j$ and the general solution is complete.

$$Y = Ap^{-j} + Bp^{j+1}$$

But when $p \to 0$ the first term is out, therefore,

$$Y = Bp^{j+1} \qquad 3.14$$

is the solution for $p \to 0$

If we combine the two expressions (3.12) and (3.14) then we will have an expression for Y with the improper points eliminated.

$$\therefore Y = e^{-p/2} p^{j+1} f(p) \qquad 3.15$$

If this is put into the Y equation (3.10), the result is

$$\frac{d^2\chi}{dp^2} - \frac{\lambda(\lambda+1)}{p^2}\chi = 0 \qquad (3.13)$$

If we try a substitution

$$\chi = p^\kappa \text{ into } (3.13)$$

then

$$\kappa(\kappa-1)p^{\kappa-2} - \frac{\lambda(\lambda+1)}{p^2}p^\kappa = 0$$

or

$$\kappa(\kappa-1)p^{\kappa-2} - \lambda(\lambda+1)p^{\kappa-2} = 0$$

or $$\kappa(\kappa-1) = \lambda(\lambda+1)$$

or $$\kappa^2 - \kappa - \lambda(\lambda+1) = 0$$

$$\kappa = \frac{1 \pm \sqrt{1+4\lambda(\lambda+1)}}{2} = \frac{1 \pm \sqrt{4\lambda^2+4\lambda+1}}{2}$$

$$\kappa = \frac{1 \pm (2\lambda+1)}{2}$$

so $\kappa = \lambda + 1$ with the $+$

and $\kappa = -\lambda$ with the $-$

$\therefore \kappa = \lambda+1, -\lambda$ and the general solution is complete.

$$\chi = Ap^{-\lambda} + Bp^{\lambda+1}$$

But when $p \to 0$ the first term is only, therefore,

$$\chi = Bp^{\lambda+1} \qquad (3.14)$$

is the solution for $p \to 0$

If we combine the two expressions (3.12) and (3.14) then we will have an expression for χ with the improper points eliminated.

$$\therefore \chi = e^{-p/2}p^{\lambda+1}L(p) \qquad (3.15)$$

If this is put into the χ equation (3.10), the result is

$$pf'' + f'(j+1) + pf'(-1/2) + f(j)(j+1)p^{-1} + (j+1)f' + f(j+1)(-1/2)$$
$$+ pf(1/4) + p(-1/2)f' + f(j+1)(-1/2) + pf(1/4) + p(-1/2)f' + f(-1/2)$$
$$(j+1) + [-1/4\,(pf) - \frac{j(j+1)}{p^2}(pf) + B/p(pf)\,] = 0$$

where prime denotes differentiation with respect to p. Collecting terms

$$pf'' + [(j+1) - p/2 + (j+1) - p/2]f' + [j(j+1)p^{-1} + (j+1)(-1/2) + p/4$$
$$+ (j+1)(-1/2) - 1/4\,p - \frac{j(j+1)}{p} + B]\,f = 0$$

so

$$f'' + [\frac{2j+2}{p} - 1]\,f' + [\frac{B-j-1}{p}]\,f = 0 \qquad 3.16$$

We may effect a solution of (3.16) by expressing f in a power series

$$f = \sum a_K p^K \qquad 3.17$$

First we must test for the starting point of the series. This is done by taking the coefficient of the smallest term when 3.17 is put into (3.16). For the case $K = K^*$

$$f' = \sum a_{K^*}(K^*)p^{K^*-1}$$

and

$$f'' = \sum a_{K^*}(K^*)(K^*-1)p^{K^*-2}$$

The smallest term is K^*-2 so all we need from the joining of (3.17) and (3.16) is

$$[\sum a_{K^*}(K^*)(K^*-1)p^{K^*-2}] + [\frac{2j+2}{p} - 1]\sum a_{K^*}(K^*)p^{K^*-1} + \ldots\ldots$$

which is not needed for starting point.

$$\therefore [p^{K^*-2}][(K^*)(K^*-1) + K^*(2j+2)] = 0 \qquad 3.18$$

(3.18) is called the Indicial Equation. This equation vanishes for $K^* = 0$ and also when

$$(K^*-1) + (2j+2) = 0$$

so

$$K^* = -2j - 1$$

$\therefore K^* = 0$ or $-2j - 1$ is a starting point for the series.

The latter should be thrown out because the minus value has some explosive qualities when $p = 0$. We only use $K^* = 0$. The result of placing $f = \Sigma a_K p^K$ into the (3.16) is

$$\Sigma a_K K(K-1)p^{K-2} + \Sigma a_K K (2j+2)p^{K-2} - \Sigma a_K K p^{K-1} + \Sigma a_K (B-j-1)p^{K-1} \equiv 0$$

To change all to p^{K-1} we use $K = K+1$ in the first two expressions so

$$[a_{K+1}(K+1)(K)p^{K-1} + a_{K+1}(K+1)(2j+2)p^{K-1}] -$$

$$-[a_K K p^{K-1} - a_K (B - j - 1)p^{K-1}] \equiv 0$$

If we remove p^{K-1} then

$$(a_{K+1})[(K+1)(K) + (K+1)(2j+2)] - (a_K)[K - (B - j - 1))] \equiv 0$$

and

$$a_{K+1} = \frac{K - B + j + 1}{(K+1)(K+2j+2)} a_K \qquad 3.19$$

which is called the Recursion Formula. For well-behaved solutions f of (3.17) must be a terminating polynomial. This is true only if according to (3.19) $K = n'$ and

$$B = n' + j + 1 \qquad 3.20$$

where

$n' = 0,1,2,3 \ldots$ which means that B must be greater than zero.

n' is the radial quantum number

$$B = n \qquad 3.21$$

so $n = n' + j + 1$ where n is the total quantum number. If (3.21) is substituted into (3.9), the result is

$$B = \frac{4\pi^2 MZe^2}{ah^2} = n$$

and

$$a = \frac{2\pi i}{h}\sqrt{2ME}$$

$$\therefore E = -\frac{2\Pi^2 M Z^2 e^4}{h^2 n^2} \qquad 3.22$$

where $n = 1, 2, 3, \ldots .$

These are the same Energy Eigenvalues that were found by Bohr in 1913.

We find that there may be any value of positive energy whatsoever but negative energy takes on quantized values according to (3.22)

Pauli developed a theory whereby it was possible to incorporate the spin into the above Schrödinger Theory. Rather than dwell on this treatise, we shall wait until the formulation of Dirac's Theory where the spin is mathematically included in the equations.

The eigenfunction may be expressed as

$$\psi_{nlm}(r, \theta, \phi) = R_{nl}(r)\,\Theta_{lm}(\theta)\,\Phi_m(\phi) \qquad 3.23$$

however, for the ground state of the one electron atom $n = 1$, $m = 0$, $l = 0$, the ψ_{nlm} may be expressed as

$$\psi_{100} = R_{10}(r)$$

which shows that the probability distribution function for the electron relative to the nucleus may be expressed in terms of the Radial function alone.

That is

$$\psi_{100}\,\psi^*_{100} = R_{10}(r)\,R^*_{10}(r)$$

Due to the symmetry through the independence of the distribution concerning ϕ and θ the hydrogen atom may be pictured as a sphere. The radial distribution function may be found by integrating $\psi\psi^*$ over all space and completing the normalization

$$\therefore D_{100}(r) = \int \psi\psi^* dv = \int RR^* dv = 4\Pi r^2\, RR^* \qquad 3.24$$

$$\therefore E = -\frac{2\pi^2 m e^4 Z^2}{h^2 n^2} \qquad 3.22$$

where $n = 1, 2, 3, \ldots$

These are the same Energy Eigenvalues that were found by Bohr in 1913.

We find that there may be any value of positive energy whatsoever, but negative energy takes on quantized values according to (3.22)

Pauli developed a theory whereby it was possible to incorporate the spin into the above Schrödinger Theory. Rather than dwell on this treatise, we shall wait until the formulation of Dirac's Theory where the spin is mathematically included in the equations.

The eigenfunction may be expressed as

$$\psi_{nlm}(r, \theta, \phi) = R_{nl}(r) \Theta_{lm}(\theta) \Phi_m(\phi) \qquad 3.23$$

However, for the ground state of the one electron atom $n = 1$, $l = 0$, $m = 0$, the ψ_{nlm} may be expressed as

$$\psi_{100} = R_{10}(r)$$

which shows that the probability distribution function for the electron relative to the nucleus may be expressed in terms of the Radial function alone.

That is

$$\psi_{100} \psi^*_{100} = R_{10}(r)\, R^*_{10}(r)$$

Due to the symmetry through the independence of the distribution concerning ϕ and θ the hydrogen atom may be pictured as a sphere. The radial distribution function may be found by integrating $\psi\psi^*$ over all areas and equating the normalization

$$\therefore D_{100}(r) = \int \psi\psi^* dv = \int R R^* dv = 4\pi r^2 R R^* \qquad 3.24$$

$D_{100}(r)dr$ being the probability that the electron lies between the r and r + dr distances from the nucleus.

By this method we have designated the "size" of the Hydrogen Atom, and we find that it approximates the size found by the Bohr Theory.

Stationary Perturbations

The next case to be considered is when a small perturbation is applied to a system so that there are small changes in the discrete energy levels of that system. An example of this might best be shown in the polarizability of the normal state in Atomic Hydrogen. When an electric field is applied to the atom in a given direction, the atoms assume a definite position causing a shift in the spectral lines. To find the change in the energy, we must develop the Rayleigh-Schrödinger Perturbation Theory.

Rayleigh-Schrödinger Perturbation

This theory will be for a time-independent non-degenerate system, a condition which would exist if an electric field were applied to the ground state of the Hydrogen Atom.

We have just completed solution of the unperturbed system

$$H_o\psi_n^o = E_n^o\psi_n^o \qquad 4.1$$

where H_o is the "unperturbed" Hamiltonian. However, we want to find solutions and eigenvalues of

$$H\psi_n = E_n\psi_n \qquad 4.2$$

where H is only a little different from H_o so

$$H = H_o + \lambda H' + \lambda^2 H'' + \cdots$$

where λ is the parameter and when $\lambda \to 0$ it reduces to $H_o\psi_n^o - E_n^o\psi_n^o = 0$

The perturbation is the $\lambda H' + \lambda H'' + \cdots$

The E_n and the ψ_n can be expanded into a power series where the ψ_n's form orthogonal sets. As in the case of the Stark Effect all the E_n's are different so we have a non-generate case.

$$\psi_n = \psi n^\circ + \lambda \psi n' + \lambda^2 \psi_n^2 + \ldots \qquad 4.3$$

$$E_n = E_n^\circ + \lambda E_n' + \lambda^2 E_n^2 + \ldots \qquad 4.4$$

If the perturbation is really a small one the terms of these series will become rapidly smaller as we consider larger powers of λ and the series will converge. Putting these expanded terms into the Schrödinger Equation.

$$[H_o + \lambda H'][\psi_n^\circ + \lambda \psi_n' + \lambda^2 \psi_n^2 + \ldots] =$$
$$[E_n^\circ + \lambda E_n' + \lambda^2 E_n^2 + \ldots][\psi_n^\circ + \lambda \psi_n' + \ldots] \qquad 4.5$$

Equating coefficients of λ:

$$H_o \psi_n^\circ = E_n^\circ \psi_n^\circ$$
$$(H' \psi_n^\circ + H_o \psi n') = (E_n^\circ \psi_n' + E_n' \psi_n^\circ) \qquad 4.6$$
$$(H_o \psi_n^2 + H' \psi_n') = (E_n^\circ \psi_n^2 + E_n' \psi_n' + E_n^2 \psi_n^\circ) \qquad 4.7$$

The unknown function ψ_n' can be expanded in terms of the known function ψ_m°

$$\psi_n' = \sum_m a_m \psi_m^\circ \qquad 4.8$$

where a_m are coefficients to be determined. (4.6) may be written by rearranging terms as

$$(H_o - E_n^\circ)\psi_n' = E_n' \psi_n^\circ - H' \psi_n^\circ \qquad 4.9$$

However
$$H' \psi_n^\circ = \alpha_{1n}^{(1)} \psi_1^\circ + \alpha_{2n}^{(1)} \psi_2^\circ + \ldots$$
$$+ \alpha_{mn}^{(1)} \psi_m^\circ + \ldots \qquad 4.10$$

and if we multiply by the complex conjugate and integrate over all space

$$\int \psi_m^{o*} H' \psi_n^o \, dv = \alpha'_{mn} = H'_{mn}$$

so (4.9) may be written

$$H' \psi_n^o = H_{1n}^{(1)} \psi_1^{(o)} + H_{2n}' \psi_2^o + \ldots = \Sigma_m H'_{mn} \psi_m^o \qquad 4.11$$

Put (4.8) and (4.11) in (4.9)

$$(H_o - E_n^o) \Sigma_m a_m \psi_m^o = E_n' \psi_n^o - \Sigma_m H'_{mn} \psi_m^o$$

When this is expanded

$$\Sigma a_m H_o \psi_m^o - E_n^o \Sigma_m a_m \psi_m^o = E_n' \psi_n^o - \Sigma_m H'_{mn} \psi_m^o \qquad 4.12$$

But the unperturbed solved equation is

$$H_o \psi_m^o = E_m^o \psi_m^o \qquad 4.13$$

Put this in (4.12) so

$$\Sigma a_m E_m^o \psi_m^o - E_n^o \Sigma_m a_m \psi_m^o = E_n' \psi_n^o - \Sigma_m H'_{mn} \psi_m^o$$

and

$$\Sigma a_m (E_m^o - E_n^o) \psi_m^o = E_n' \psi_n^o - \Sigma_m H'_{mn} \psi_m^o \qquad 4.14$$

When m = n the coefficient of ψ_n^o is

$$0 = E_n' - H_{nn}'$$

and

$$E_n' = H_{nn}' = \int \psi_n^{o*} H' \psi_n^o \, dv \qquad 4.15$$

This is the first order correction under the perturbation theory. Our next problem is to find the coefficient of the expanded ψ_m^o. We find this by the process of normalization.

$$\text{If } \psi_n = \psi_n^o + \lambda \psi_n' + \lambda^2 \psi_n^2 + \ldots$$

$$\psi_m^* = \psi_m^{o*} + \lambda \psi_m'^* + \lambda^2 \psi_m^2 +$$

To normalize

$$1 = \int \psi_m^* \psi_n \, dv = \int \psi_m{}^{o*} \psi_n{}^{o} \, dv + \lambda[\int \psi_m{}^{o*} \psi_n' \, dv + \int \psi_m'^{*} \psi_n{}^{o} \, dv] + \lambda^2[\,]$$

Since

ψ_m^*, ψ_n and ψ_m^{o*}, $\psi_n{}^{o}$ are each orthogonal sets. If $\psi_m^* \psi_n$ or $\psi_m{}^{o*} \psi_n{}^{o}$ are integrated over all space and normalized, all terms of the expansion will be zero except when $m = n$. Upon insertion of (4.8) we find

$$1 = 1 + \lambda[\int \psi_m{}^{o*} \sum_m a_m \psi_m{}^{o} \, dv + \int \Sigma \psi_n{}^{o*} a_n \psi_n{}^{o} \, dv)]$$

Where

$$\sum_m a_m \psi_m{}^{o} \psi_m = a_1 \psi_m{}^{o} \psi_1{}^{o} + a_2 \psi_m{}^{o} \psi_2{}^{o} + \ldots . a_m \psi_m{}^{o} \psi_m{}^{o}$$

and when $m = n$ only the last term remains

so

$$1 = 1 + \lambda[2a_n] +$$

$$2\lambda a_n = 0$$

$$a_n = 0$$

so all coefficient yield a value except when $m = n$. When m does not equal n then from (4.14)

Coefficient of $\psi_m{}^{o}$ when $m \neq n$	$a_m(E_m^o - E_m^o) = - H'_{mn}$
	so $a_m = - \dfrac{H'_{m_n}}{E_m{}^{o} - E_n{}^{o}}$

so now (4.8) is

$$\psi_{n'} = \sum_m' - \frac{H'_{mn}}{E_m{}^{o} - E_n{}^{o}} \psi_m{}^{o} \qquad 4.16$$

where Σ' means that n term is missing as proved above.

To get the second order perturbation we arrange (4.7) as follows

$$(H_o - E_n{}^{o}) \psi_n{}^{2} = E_n{}^{2} \psi_n{}^{o} + E_n' \psi_{n'} - H' \psi_n{}' \qquad 4.17$$

If we expand $\psi_n{}^{2}$ as we did $\psi_n{}'$

$$\psi_n^{2} = \sum_m \beta_m \psi_m^{\circ} \qquad 4.18$$

If we put this in (4.17) along with the values for E_n' and ψ_n' already computed we get

$$(H_o - E_n^{\circ})\sum_m \beta_m \psi_m^{\circ} = E_n^{(2)}\psi_n^{\circ} + \sum_m{}' \frac{H'_{mn} H'_{nn}}{E_n^{\circ} - E_m^{\circ}} \psi_m^{\circ} - H'\psi_n' \qquad 4.19$$

However $H'\psi_n'$ may be expressed as follows

$$H'\psi_n' = \sum_m{}' \frac{H'_{mn}}{E_n^{\circ} - E_m^{\circ}} H'\psi_m^{\circ}$$

but

$$H'\psi_m^{\circ} = \sum H'_{mn}\psi_n^{\circ}$$

so

$$H'\psi_n' = \sum_m{}' \frac{H'_{mn}}{E_n^{\circ} - E_m^{\circ}} \sum_K H'_{Km}\psi_K^{\circ}$$

$$= \sum_m{}' \sum_K \frac{H'_{mn}}{E_n^{\circ} - E_m^{\circ}} H'_{Km}\psi_K^{\circ}$$

Putting this and $H_o\psi_m^{\circ} = E_m^{\circ}\psi_m^{\circ}$ in (4.19)

$$(E_m^{\circ} - E_n^{\circ})\beta_m\psi_m^{\circ} = E_n^{2}\psi_n^{\circ} + \sum_m{}' \frac{H'_{nn} H'_{mn}}{(E_n^{\circ} - E_m^{\circ})}\psi_m^{\circ} - \sum_m{}' \sum_K \frac{H'_{mn} H'_{Km}}{E_n^{\circ} - E_m^{\circ}}\psi_K^{\circ}$$

When $K = n$ the coefficient of ψ_n° is

$$0 = E_n^{2} - \sum_m{}' \frac{H'_{mn} H'_{nm}}{(E_n^{\circ} - E_m^{\circ})}$$

$$E_n^{2} = \sum_m{}' \frac{H'_{mn} H'_{nm}}{(E_n^{\circ} - E_m^{\circ})} \qquad 4.20$$

which is correction for second order perturbation.

$$\psi^n_2 = \sum_m c^n_m \psi^m_o \qquad (4.18)$$

If we put this in (4.17) along with the values for E^n_1 and ψ^n_1 already computed we get

$$(H^o - E^n_o)\sum_m c^n_m \psi^m_o = E^n_{(2)}\psi^n_o + \sum_i \frac{H_{in} H_{ni}}{E^n_o - E^m_o} c^n_m \psi^m_o - H_{1i}\psi^n_1 \qquad (4.19)$$

However $H_{1i}\psi^n_1$ may be expressed as follows

$$H_{1i}\psi^n_1 = \sum_m \frac{}{E^n_o - E^m_o} H_{1i}\psi^m_o$$

but

$$H_{1i}\psi^n_o = \sum H_{1m}\psi^n_o$$

so

$$H_{1i}\psi^n_1 = \sum_m \frac{}{E^n_o - E^m_o} \sum_K H_{1m} c^K_n \psi^K_o$$

$$= \sum_K \sum_m \frac{H_{1m}}{E^n_o - E^m_o} H_{1m} c^K_n \psi^K_o$$

Putting this and $H^o\psi^m_o = E^m_o\psi^m_o$ in (4.19)

$$(E^n_o - E^m_o)\sum_m c^n_m \psi^m_o = E^n_{(2)}\psi^n_o + \sum_i \frac{H_{1m} H_{1n}}{(E^n_o - E^m_o)} \psi^m_o - \sum_K \sum_i \frac{H_{1m} H_{1n}}{E^n_o - E^m_o} c^K_n \psi^K_o$$

When $K = n$ the coefficient of ψ^n_o is

$$0 = E^n_2 - \sum_i \frac{H_{1n} H_{1n}}{(E^n_o - E^n_o)}$$

$$E^n_2 = \sum_i \frac{H_{1n} H_{1n}}{(E^n_o - E^n_o)} \qquad (4.20)$$

Which is correction for second order perturbation.

The value of E_n up to the second order of perturbation is

$$E_n = E_n^o + \lambda H'_{nn} + \lambda^2 \sum_m{}' \frac{H'_{nm}\ H'_{mn}}{(E_n^o - E_m^o)} \qquad 4.21$$

With this developed Rayleigh-Schrödinger perturbation formula we are able to easily solve to a fair approximation a non-degenerate case, such as the Stark Effect.

Polarizability

The wave equation for a hydrogen atom in an electric field can be written as

$$-\frac{h^2}{8\pi^2 M}\nabla^2\psi - \frac{Ze^2}{r}\psi + eD\,\mathrm{X}\,\psi = E_n\psi \qquad 5.1$$

where

$$H_o = -\frac{h^2}{8\pi^2 M}\nabla^2 - \frac{Ze^2}{r} \quad \text{is the unperturbed state}$$

$\lambda H' = eD\mathrm{X}$ is the perturbation to be expanded in terms of D where e is the charge on the electron and M is the reduced mass, and $eD\mathrm{X}$ represents the interaction with an electric field of strength D along the X axis.

Using the Rayleigh-Schrödinger equation

$$E_n = E_n^o + eD\int\psi_n^o\,\mathrm{X}\,\psi_n^o\,dv + e^2D^2\sum_m{}'\frac{X_{nm}\,X_{mn}}{(E_n^o - E_m^o)}$$

Since $-X_{nm} = X_{mn}$

and

$$X_{nn} = \int\psi_n^o\,\mathrm{X}\,\psi_n^o\,dv$$

$$X_{nm} = \int\psi_n^o\,\mathrm{X}\,\psi_m^o\,dv$$

we have

$$E_n = E_n^o + eD\mathrm{X}_{nn} + e^2D^2\sum_m{}'\frac{|X_{nm}|^2}{(E_m^o - E_n^o)} \qquad 5.2$$

When the hydrogen atom is in its ground state, that is n = 1 the following energy relation holds from (5.2)

The value of E_n up to the second order of perturbation is

$$E_n = E_n^0 + \lambda H'_{nn} + \lambda^2 \sum_m \frac{H'_{nm} H'_{mn}}{(E_n^0 - E_m^0)} \qquad 4.22$$

With this developed Rayleigh-Schrödinger perturbation formula we are able to easily solve to a fair approximation a non-degenerate case, such as the Stark Effect.

Polarizability

The wave equation for a hydrogen atom in an electric field can be written as

$$-\frac{\hbar^2}{8\pi^2 M} \nabla^2 \psi - \frac{2e^2}{r} \psi + eD\chi \psi = E\psi \qquad 5.1$$

where

$$H^0 = -\frac{\hbar^2}{8\pi^2 M} \nabla^2 - \frac{2e^2}{r} \quad \text{is the unperturbed state}$$

$H' = eD\chi$ is the perturbation to be expanded in terms of

D where e is the charge on the electron and M is the reduced mass, and $eD\chi$ represents the interaction with an electric field of strength D along the χ axis.

Using the Rayleigh-Schrödinger equation

$$E_n = E_n^0 + eD \int \psi_n^0 \chi \psi_n^0 \, dv + e^2 D^2 \sum_m \frac{X_{nm} X_{mn}}{(E_n^0 - E_m^0)}$$

Since $-X_{nm} = X_{mn}$

and

$$X_{nn} = \int \psi_n^0 \chi \psi_n^0 \, dv$$

$$X_{nn} = \int \psi_n^0 \chi \psi_n^0 \, dv$$

we have

$$E_n = E_n^0 + eD\chi_{nn} + e^2 D^2 \sum_m \frac{|X_{nm}|^2}{(E_n^0 - E_m^0)} \qquad 5.2$$

When the hydrogen atom is in its ground state, that is $n = 1$ the following energy relation holds from (5.2)

$$E_1 = E_1^o + eDX_{11} + e^2D^2 \sum_m{}' \frac{|x_{1m}|^2}{(E_m^o - E_1^o)} \qquad 5.3$$

In this case the first order eDX_{11} vanishes because $|\psi_1|^2$ is an even function of x.

In classical physics it has been found that the small amount of energy of an atom due to static electric field is

$$\Delta E = -1/2 \propto D^2 \qquad 5.4$$

where $\propto$ is the polarizibility.

Making a comparison with (5.3)

$$\Delta E_1 = E_1 - E_1^o = -1/2 \left(2e^2 \sum_m{}' \frac{|x_{1m}|^2}{(E_m^o - E_1^o)}\right) D^2$$

or the polarizability of our atom as solved above is

$$\propto = 2e^2 \sum_m{}' \frac{|x_{1m}|^2}{(E_m^o - E_1^o)} \qquad 5.5$$

There will be a small change in the eigenfunction which may be expressed as new eigenfunction for the perturbed system. These are the expanded ψ's used in the building of the Rayleigh-Schrödinger Theory.

The new energy eigenvalue expressed in terms of the energy found in (3.22) is

$$E_1 = -\frac{2\pi^2 Me^4}{h^2} + e^2D^2 \sum_m{}' \frac{|X_{1m}|^2}{h\nu_{m1}}$$

Building a Linear Hamiltonian for a Dirac Electron

Our work in this theory will bring us into contact with relativity and electron spin. In considering that the electron is traveling in a purely electrostatic field we have imposed so serious restrictions upon the system, because in reality a field that is purely electrostatic from the standpoint of one observer may have a magnetic field with respect to another

observer moving relative to the first.

If the total energy of the electron is a summation of the kinetic, potential and rest energies then

$$E = T + V + M_e c^2 \qquad 6.1$$

where M_e is the rest mass of the electron and c is equal to the velocity of light. (6.1) may be transformed to

$$\frac{(E - V)^2}{c^2} = p^2 + M_e^2 c^2$$

where p is the momentum which has the components p_x, p_y, p_z, and $= \frac{M_e V}{\sqrt{1 - \frac{V^2}{c^2}}}$

Solving for E we have

$$E = V \pm c\sqrt{p_x^2 + p_y^2 + p_z^2 + M_e^2 c^2}$$

and if H is substituted for E, the result is the Hamiltonian

$$H = V \pm c\sqrt{p_x^2 + p_y^2 + p_z^2 + M_e c^2} \qquad 6.2$$

where the positive sign is used in the theory of positrons. At present we will confine ourselves to the use of the negative equation.

Even before this Hamiltonian had been developed, work on proposed relativistic generalizations in the Schrödinger equation had shown that partial differential equations of the second order in the time variable t were present, whereas the simple Schrödinger equation involved the first derivative of t with respect to the time. That is

$$H\psi = \frac{ih}{2\pi}\frac{\partial \psi}{\partial t} \qquad 6.3$$

Dirac proposed that these second order coefficients must be changed to those of the first order to complete a successful theory. The two main reasons for this intuition was that $\psi\psi^*$ function or the probability density is not necessarily positive using a relativistic Schrödinger approach, a condition which must be true and also that $\partial^2\psi/\partial t^2$ term implies that

you not only have to specify for ψ but also $\partial\psi/\partial t$ at some given time. Such a situation should be avoided if possible.

If we insert momenta operators

$$p_k = \frac{h}{2\pi i}\frac{\partial}{\partial k} \quad \text{where } k = (x, Y, Z)$$

in (6.2) we have

$$H = V - c\sqrt{-\left(\frac{h}{2\pi}\right)^2\left(\frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial Y^2} + \frac{\partial^2}{\partial Z^2}\right) + M_e{}^2c^2} \qquad 6.4$$

Since this quadratic operator upsets the whole scheme of Quantum Mechanics, as previously mentioned, it was necessary for Dirac to Linearize the H. If we can get the radical to a perfect square we will have accomplished this. This can be done as follows:

$$(p_x{}^2 + p_y{}^2 + p_z{}^2 + M_e{}^2c^2) =$$

$$(\alpha_x p_x + \beta_y p_y + \beta_z p_z + \alpha_m M_e c)^2$$

where

$\beta_x, \beta_y, \beta_z, \beta_m$ are left undetermined at present.

Carrying out the multiplication we get

$$(\beta_x p_x + \beta_y p_y + \beta_z p_z + \beta_m M_e c)^2$$

$$= \beta_x{}^2 p_x{}^2 + \beta_x\beta_y p_x p_y + \beta_x\beta_z p_x p_z + \beta_x\beta_m p_x M_e c$$

$$+ \beta_y\beta_x p_y p_x + \beta^2{}_y p_y{}^2 + \beta_y\beta_z p_y p_z + \beta_y\beta_m p_y M_e c$$

$$+ \beta_z\beta_x p_z p_x + \beta_z\beta_y p_z p_y + \beta_z{}^2 p^2{}_z + \beta_z\beta_m p_z M_e c$$

$$+ \beta_m\beta_x M_e c p_x + \beta_m\beta_y M_e c p_y + \beta_m\beta_z M_e c p_z + \beta_m{}^2 M_e{}^2 c^2$$

If we designate the α as operators which anticommute then

$$\alpha_x\alpha_y + \alpha_y\alpha_x = 0 \qquad \alpha_x\alpha_z + \alpha_z\alpha_x = 0 \qquad \alpha_x\alpha_m + \alpha_m\alpha_x = 0$$

$$\alpha_y\alpha_z + \alpha_z\alpha_y = 0 \qquad \alpha_y\alpha_m + \alpha_m\alpha_y = 0 \qquad \alpha_z\alpha_m + \alpha_m\alpha_z = 0$$

and since the p's commute with one another we have

$$\alpha_x^2 p_x^2 + \alpha_y^2 p_y^2 + \alpha_z^2 p_z^2 + \alpha_m^2 M_e^2c^2 = (\alpha_x p_x + \alpha_y p_y + \alpha_z p_z + \alpha_m mc)^2$$

and everything is satisfied if we further demand that

$$\alpha_x^2 = \alpha_y^2 = \alpha_z^2 = \alpha_m^2 = 1$$

so $H = V - c\alpha_x p_x - c\alpha_y p_y - c\alpha_z p_z - \alpha_m M_e c^2$

and if we put in the operators of the p's $p_k = \frac{-i\,h}{2\pi}\frac{\partial}{\partial k}$

$$H = V + c\alpha_x \frac{hi}{2\pi}\frac{\partial}{\partial x} + c\alpha_y \frac{hi}{2\pi}\frac{\partial}{\partial y} + c\alpha_z \frac{hi}{2\pi}\frac{\partial}{\partial z} - \alpha_m M_e c^2 \qquad 6.5$$

This is the famous linear operator, the celebrated Dirac Hamiltonian for an electron in an electrostatic field.

Using the four by four matrices of Dirac

$$\alpha_x = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \qquad \alpha_y = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \qquad 6.6$$

$$\alpha_z = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \quad ; \quad \alpha_m = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

Considering that the Dirac Operators have four by four matrices, the Dirac ψ-function ψ must have the form

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} \qquad 6.7$$

The Hydrogen-Like Atom

The equation of motion not involving time is $H\psi = E\psi$

Substituting for H

$$(V - c\alpha_x p_x - c\alpha_y p_y - c\alpha_z p_z - \alpha_m M_e c^2)\psi = E\psi \qquad 7.1$$

Replacing α's by matrices and multiplying V by a unitary matrix

$$\left[V \begin{pmatrix} 1&0&0&0 \\ 0&1&0&0 \\ 0&0&1&0 \\ 0&0&0&1 \end{pmatrix} - c \begin{pmatrix} 0&0&0&1 \\ 0&0&1&0 \\ 0&1&0&0 \\ 1&0&0&0 \end{pmatrix} p_x - c \begin{pmatrix} 0&0&0&-i \\ 0&0&i&0 \\ 0&-i&0&0 \\ i&0&0&0 \end{pmatrix} p_y - c \begin{pmatrix} 0&0&1&0 \\ 0&0&0&-1 \\ 1&0&0&0 \\ 0&-1&0&0 \end{pmatrix} p_z \right.$$

$$\left. - \begin{pmatrix} 1&0&0&0 \\ 0&1&0&0 \\ 0&0&-1&0 \\ 0&0&0&-1 \end{pmatrix} M_e c^2 \right] \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}$$

$$\left[\begin{pmatrix} V&0&0&0 \\ 0&V&0&0 \\ 0&0&V&0 \\ 0&0&0&V \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} - \begin{pmatrix} 0&0&0&cpx \\ 0&0&cpx&0 \\ 0&cpx&0&0 \\ cpx&0&0&0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} - \begin{pmatrix} 0&0&0&-icpy \\ 0&0&icpy&0 \\ 0&-icpy&0&0 \\ icpy&0&0&0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} \right.$$

$$\left. - \begin{pmatrix} 0&0&cpz&0 \\ 0&0&0&-cpz \\ cpz&0&0&0 \\ 0&-cpz&0&0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} - \begin{pmatrix} Mc^2&0&0&0 \\ 0&Mc^2&0&0 \\ 0&0&-Mc^2&0 \\ 0&0&0&-Mc^2 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} \right] = E \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}$$

$$\left[\begin{pmatrix} V\psi_1 \\ V\psi_2 \\ V\psi_3 \\ V\psi_4 \end{pmatrix} - \begin{pmatrix} cp_x\psi_4 \\ cp_x\psi_3 \\ cp_x\psi_2 \\ cp_x\psi_1 \end{pmatrix} - \begin{pmatrix} -icp_y\psi_4 \\ icp_y\psi_3 \\ -icp_y\psi_2 \\ icp_y\psi_1 \end{pmatrix} - \begin{pmatrix} cp_z\psi_3 \\ -cp_z\psi_4 \\ cp_z\psi_1 \\ -cp_z\psi_2 \end{pmatrix} - \begin{pmatrix} M_ec^2\psi_1 \\ M_ec^2\psi_2 \\ -M_ec^2\psi_3 \\ -M_ec^2\psi_4 \end{pmatrix}\right]$$

$$= E\begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}$$

$$\left.\begin{aligned} (V - M_ec^2)\psi_1 - cp_z\psi_3 - c(p_x - ip_y)\psi_4 &= E\psi_1 \\ (V - M_ec^2)\psi_2 + cp_z\psi_4 - c(p_x + ip_y)\psi_3 &= E\psi_2 \\ (V + M_ec^2)\psi_3 - cp_z\psi_1 - c(p_x - ip_y)\psi_2 &= E\psi_3 \\ (V + M_ec^2)\psi_4 + cp_z\psi_2 - c(p_x + ip_y)\psi_1 &= E\psi_4 \end{aligned}\right\} \quad 7.2$$

If we replace p_x by $\frac{-ih}{2\pi}\partial/\partial x$, and so on, and after a slight rearrangement we get the equation

$$\left.\begin{aligned} 2\pi i/h\,(E/c - V/c + M_ec)\psi_1 + (\partial/\partial x - i\,\partial/\partial y)\psi_4 + \partial/\partial z\,\psi_3 &= 0 \\ 2\pi i/h\,(E/c - V/c + M_ec)\psi_2 + (\partial/\partial x + i\,\partial/\partial y)\psi_3 - \partial/\partial z\,\psi_4 &= 0 \\ 2\pi i/h\,(E/c - V/c - M_ec)\psi_3 + (\partial/\partial x - i\,\partial/\partial y)\psi_2 + \partial/\partial z\,\psi_1 &= 0 \\ 2\pi i/h\,(E/c - V/c - M_ec)\psi_4 + (\partial/\partial x + i\,\partial/\partial y)\psi_1 - \partial/\partial z\,\psi_2 &= 0 \end{aligned}\right\} \quad 7.3$$

We see that the Dirac equation is in itself four partial differential equations. These may be solved simultaneously for the ψ's.

Solution of Dirac's Radial Equations for Central Field

If we make the designation that

$$\alpha_x = \rho_1\sigma_x\,; \quad \alpha_y = \rho_1\sigma_y\,; \quad \alpha_z = \rho_1\sigma_z$$

$$\alpha_m = \rho_3 \qquad 8.1$$

The Dirac equation (6.5) may be written as

$$H = V - c\rho_1 (\sigma_x p_x + \sigma_y p_y + \sigma_z p_z) - \rho_3 M_e c^2$$

where

$$\sigma_x = \begin{pmatrix} 0&1&0&0 \\ 1&0&0&0 \\ 0&0&0&1 \\ 0&0&1&0 \end{pmatrix} \sigma_y = \begin{pmatrix} 0&-i&0&0 \\ i&0&0&0 \\ 0&0&0&-i \\ 0&0&i&0 \end{pmatrix} \sigma_z = \begin{pmatrix} 1&0&0&0 \\ 0&-1&0&0 \\ 0&0&1&0 \\ 0&0&0&-1 \end{pmatrix}$$

$$\rho_1 = \begin{pmatrix} 0&0&1&0 \\ 0&0&0&1 \\ 1&0&0&0 \\ 0&1&0&0 \end{pmatrix} \rho_2 = \begin{pmatrix} 0&0&-i&0 \\ 0&0&0&-i \\ 1&0&0&0 \\ 0&i&0&0 \end{pmatrix} \rho_3 = \begin{pmatrix} 1&0&0&0 \\ 0&1&0&0 \\ 0&0&-1&0 \\ 0&0&0&-1 \end{pmatrix} \qquad 8.3$$

The ρ_2 does not need to be included until we work with the electromagnetic field.

Under Dirac's theory by means of the Commutator Bracket we find the orbital angular momentum $\bar{L}$ is not a constant of motion for the case as found in the Classical Theory using the Poisson Bracket. Here a component of $\bar{L}$, say L_x, gives this relation when placed in a bracket with H.

$$[L_x, H] = L_x H - H L_x = - \frac{ih}{2\pi} c\rho_1 (\sigma_y p_z - \sigma_z p_y) \neq 0 \qquad 8.4$$

We find that the commutation of the σ's with H give 8.5

$$[\sigma_x, H] = \sigma_x H - H\sigma_x = 2ic\rho_1 (\sigma_y p_z - \sigma_z p_y)$$

Therefore the relationship between (8.4) and (8.5) is

$$L_x H - H L_x = - \frac{h}{4\pi} (\sigma_x H - H\sigma_x) \quad \underline{\text{or}} \quad (L_x + \frac{h}{4\pi}\sigma_x)H - H(L_x + \frac{h}{4\pi}\sigma_x) = 0$$

$$\underline{\text{or}} \quad [(L_x + \frac{h}{4\pi}\sigma_x), H] = 0 \qquad 8.6$$

$\therefore L_x + \frac{h}{4\pi}\sigma_x$ is a constant of motion in the Dirac theory. It was found that the added term $\frac{h}{4\pi}\sigma_x$ was just equal to the value attributed to the electron spin by Uhlenbeck and Goudsmit .

$\therefore \bar{S} = \frac{h}{4\pi}\bar{\sigma}$ is spin angular momentum and the total angular momentum is

$$\overline{J} = \overline{L} + \overline{S}$$

Using the constants of motion for the central field, namely

$$J_z,\ J^2 \text{ and } K$$

where

$$K = \gamma_m \left(\frac{8\pi^2}{h^2} \overline{L}\cdot\overline{S} + 1 \right)$$

and restricting ourselves to the use of eigenfunctions that would be eigenfunctions for the constants and H we find that Dirac's four equations break down into two radial equations.

$$\left.\begin{aligned} (E + M_e c^2 - V)F - \frac{hc}{2\pi}\frac{dG}{dr} - \frac{hck}{2\pi r} G &= 0 \\ (E + M_e c^2 - V)G + \frac{hc}{2\pi}\frac{dF}{dr} - \frac{hck}{2\pi r} F &= 0 \end{aligned}\right\} \qquad 8.7$$

Where the two radial functions are expressed as

$$R_F = r^{-1} F$$

$$R_G = r^{-1} G$$

and k is the eigenvalue of K and ranges.

$$k = \pm 1\ ;\ \pm 2\ ;\ \pm 3$$

If we let

$$a_1 = \frac{2\pi(M_e c^2 + E)}{hc} \quad \text{and} \quad a_2 = \frac{2\pi(M_e c^2 - E)}{hc} \qquad 8.8$$

and $p = ar$ then $a = +\sqrt{a_1 a_2} = \dfrac{2\pi(M_e^2 c^4 - E^2)^{1/2}}{hc}$

On substitution of the potential for the central field $V = -\dfrac{e^2}{r}$ into equations (8.7) we are able to use the fine structure constant

$$\gamma = \frac{2\pi e^2}{hc} \qquad 8.9$$

where $\gamma \sim \frac{1}{137}$ which checks with Eddington's value.

(8.7) may be written as

$$\begin{aligned} a_1 F + 1/r(\gamma F - kG) - dG/dr &= 0 \\ a_2 G + 1/r(-\gamma G + kF) - dF/dr &= 0 \end{aligned} \qquad 8.10$$

We complete the solution by following a somewhat similar path as was used in the solving of the non-relativistic radial equations in the Schrödinger method.

By making the change in variable from r to p the following equations result

$$\frac{dG}{dp} + \frac{kG}{p} - \frac{a_1 F}{a} - \frac{\alpha F}{p} = 0$$

$$\frac{dF}{dp} - \frac{kF}{p} - \frac{a_2 G}{a} + \frac{\alpha G}{p} = 0 \qquad 8.11$$

We let

$$F(p) = f(p)e^{-p};\ G(p) = g(p)e^{-p} \qquad 8.12$$

and the equation for f and g are

$$\frac{dg}{dp} - g + \frac{kg}{p} - \left(\frac{a_1}{a} + \frac{\alpha}{p}\right) f = 0$$

$$\frac{df}{dp} - f - \frac{kf}{p} - \left(\frac{a_2}{a} - \frac{\alpha}{p}\right) g = 0 \qquad 8.13$$

We look for solutions in the form of a power series namely 8.14

$$f = c_s p^s \text{ and } g = b_s p^s \text{ where } s = s^* ;\ s^* + 1;\ s^* + 2$$

If we let $s = s^*$ we can determine the starting points of the series by substituting (8.14) into (8.13) and setting up equations of the coefficients of the lowest term p^{s^*-1}

then

$$S^* b_{s^*} + k b_{s^*} - \alpha c_{s^*} = 0$$

$$S^* c_{s^*} - k c_{s^*} + \alpha b_{s^*} = 0 \qquad 8.15$$

These are called the Indicial Equations. These two homogeneous equations for b_s and c_s have non-vanishing solutions if and only if the determinantal

equation

$$\begin{vmatrix} \alpha & -(s^* + k) \\ (s^* - k) & \alpha \end{vmatrix} = 0$$

$$s^* = \pm (h^2 - \alpha^2)^{1/2} \qquad 8.16$$

We use only the plus term for the negative term has explosive qualities resulting in F and G being ill-behaved at the origin.

Substituting (8.14) into (8.13) and equating coefficients of p^{s-1} we find

$$(s + k)b_s - \alpha c_s - b_{s-1} - (a_1/a)\, c_{s-1} = 0$$

$$(s - k)c_s + \alpha b_s - c_{s-1} - (a_2/a)\, b_{s-1} = 0 \qquad 8.17$$

Multiply both through by a and

$$\begin{aligned} a(s + k)b_s - \alpha a c_s - a b_{s-1} - a_1 c_{s-1} &= 0 \\ a(s - k)c_s + \alpha a b_s - a c_{s-1} - a_2 b_{s-1} &= 0 \end{aligned} \qquad 8.18$$

Multiplying the top by a and the bottom one by a_1 and then using the relationship from (8.8) that $a = \sqrt{a_1 a_2}$

$$a^2(s+k)b_s - \alpha a^2 c_s - a^2 b_{s-1} - a a_1 c_{s-1} = 0$$

$$a a_1 (s-k)c_s + \alpha a a_1 b_s - a a_1 c_{s-1} - a_1 a_2 b_{s-1} = 0$$

Subtracting one from the other results in the elimination of s-1 terms.

$$a^2(s+k)b_s - a a_1 (s-k)c_s - \alpha a^2 c_s - \alpha a a_1 b_s = 0 \qquad 8.19$$

or

$$a_2(s+k)b_s - a(s-k)c_s - \alpha a_2 c_s - \alpha a b_s = 0$$

When the c's and b's of (8.14) have large values of s then (8.19) reduces to

$$a_2 b_s \cong a c_s \qquad 8.20$$

We may eliminate the b's from the bottom of (8.19) by using (8.20)

$$a(s-k)c_s + \gamma\frac{a^2 c_s}{a_2} - ac_{s-1} - \frac{a_2 a}{a_2}c_{s-1} \cong 0$$

$$a(s-k)c_s + \alpha a_1 c_s - ac_{s-1} - ac_{s-1} \cong 0$$

$$(a(s-k) + \alpha a_1)c_s - 2ac_{s-1} \cong 0$$

and since s is large

$$asc_s - 2ac_{s-1} \cong 0$$

or
$$\frac{c_s}{c_{s-1}} \cong \frac{2}{s} \qquad 8.21$$

and in a similar method

$$\frac{b_s}{b_{s-1}} \cong \frac{2}{s} \qquad 8.22$$

This means that both series have the asymptotic form e^{2p} and regular solutions are obtained only if they terminate. If this occurred at $s = n'$ then $b_{n'+1} = c_{n'+1} = 0$ or any higher b or c will have the same result and according to (8.19) the series in (8.14) terminates with a term $p^{n'}$.

Since both series start with a term in p^{s^*} and the exponents of p increase by steps of unity

$$\therefore\ n' - s^* = n \quad \text{where} \quad n = |k|, |k|+1, |k|+2, \ldots$$

and by the use of (8.16)

$$n' = n - |k| + (k^2 - \gamma^2)^{1/2} \qquad 8.23$$

$$n = 1, 2, 3 \ldots.$$

$$k = \pm 1; \pm 2; \ldots. \pm(n-1), -n$$

Assuming s to be small we may write n' for s-1 in (8.18)

$$a(n'+1+k)b_{n'+1} - \alpha a c_{n'+1} - ab_{n'} - a_1 c_{n'} = 0$$

and setting $c_{n'+1}$ and $b_{n'+1}$ equal to zero because any value after n' is cut off in the series.

$$ab_{n'} = a_1 c_{n'} \qquad 8.24$$

If we eliminate $b_{n'}$ by using (8.19) then

$$2n' a_1 a^2 = (a_1^2 - a^2)\alpha$$

and by using (8.8) reduces to

$$n'(M_e{}^2c^4 - E^2)^{1/2} = E\alpha \qquad 8.25$$

or

$$E = M_e c^2[1 + (\frac{\alpha}{n'})^2]^{-1/2}$$

where n' is expressed as (8.23)

If we eliminate the rest energy $M_e c^2$ from (8.25) then

$$W = E - M_e c^2 \qquad 8.26$$

which is the Sommerfeld fine structure formula. By means of this formula, theory was able to coincide with experiment giving a good account for multiplicity of lines which were once called distinct singlets under the Bohr theory.

The eigenfunctions may be solved by methods related to solving confluent hypergeometric functions. These will not be investigated in this paper.

Examination of the Energy reveals that under this principle there would be a continuous spectrum of values above $M_e c^2$ and below $-M_e c^2$ but between these two limits only discrete values are present. By the inclusion of both positive and negative energy levels, Dirac was able to postulate his "hole" theory which allowed the theory of positrons to be developed.

B. Electromagnetic Fields

Specifications of the Potentials

With the introduction of an electromagnetic field we find that we have not only a scalar potential present, but also a vector potential, and if we except Lorentz' electron theory then these potentials may be used in conjunction with Maxwell's Equations for empty space.

In electrostatic units they are

$$\text{Curl } \bar{H} = \frac{4\pi \bar{J}}{c} \quad \frac{1}{c}\frac{\partial \bar{E}}{\partial t} \qquad 9.1$$

$$\text{Curl } \bar{E} = -\frac{1}{c}\frac{\partial \bar{H}}{\partial t} \qquad 9.2$$

$$\text{Div } \bar{E} = 4\pi\rho \qquad 9.3$$

$$\text{Div } \bar{H} = 0 \qquad 9.4$$

where ρ is the charge density; that is charge/cm^3

and $\bar{J}$ is the current density in current/cm^2

and $\bar{E}$ is the electric field strength

and $\bar{H}$ is the magnetic field strength

We are able to obtain the conservation laws for charge and current densities that will show that the total current coming out of a region is equal to the decrease in charge of the region as follows:

The total current in a region $\bar{I}$ may be thought of as the sum of two currents, the conduction current, $\bar{J}$ or current/sq.cm.; and the displacement current $\frac{1}{4\pi}\frac{\partial \bar{E}}{\partial t}$

so $$\bar{I} = \bar{J} + \frac{1}{4\pi}\frac{\partial \bar{E}}{\partial t} \qquad 9.5$$

Putting this in the (9.1) we have

$$\text{Curl } \bar{H} = \frac{4\pi}{c}\bar{I} \text{ that is } \bar{\nabla} \times \bar{H} = \frac{4\pi \bar{I}}{c}$$

Taking the divergence of both sides

$$\bar{\nabla}.\bar{\nabla} \times \bar{H} = \frac{4\pi}{c}\bar{\nabla}.\bar{I}$$

Since $(\nabla\nabla H] = 0$; because if two vectors in a scalar triple are equal the result is zero, then

$$\text{Div } \bar{I} = 0 \qquad 9.6$$

Taking the divergence of (9.5)

$$\text{Div } \bar{I} = \text{Div } \bar{J} + \frac{1}{4\pi}\frac{\partial}{\partial t} (\text{Div } \bar{E})$$

Putting in (9.3) and (9.6)

$$0 = \text{Div } \bar{J} + \frac{1}{4\pi}\frac{\partial}{\partial t}(4\pi\rho)$$

$$\text{Div } \bar{J} = -\frac{\partial \rho}{\partial t} \text{ Continuity Equation} \qquad 9.7$$

The above is the conservation law for charge and current densities. The field intensities may be expressed in terms of a scalar and vector potential as follows:

From (9.4) $\text{Div } \bar{H} = 0$ however, it would be just as well to have said $\bar{H} = \text{Curl } \bar{A}$ 9.8

where $\bar{A}$ is a vector potential because if we put this in (9.4) we get $\text{Div Curl } \bar{A} = 0$ or

$$0 = 0$$

Putting (9.8) into (9.2) we get

$$\text{Curl } \bar{E} = -\frac{1}{c}\frac{\partial}{\partial t} (\text{Curl } \bar{A}) \text{ or}$$

$$\text{Curl}(\bar{E} + \frac{1}{c}\frac{\partial \bar{A}}{\partial t}) = 0 \qquad 9.9$$

In vectors it is known that if the curl of a vector is zero then that vector may be expressed as the negative gradient of a scalar potential.

$$\therefore \bar{E} + \frac{1}{c}\frac{\partial \bar{A}}{\partial t} = -\text{ grad } \phi$$

where ϕ is in a scalar potential and

$$\bar{E} = -\frac{1}{c}\frac{\partial \bar{A}}{\partial t} - \text{grad } \phi \qquad 9.10$$

By putting (9.8) and (9.10) into (9.1) we will be able to obtain an equation which will specify the $\bar{A}$ more explicitly.

$$\text{Curl Curl } \bar{A} = \frac{4\pi\bar{J}}{c} + \frac{1}{c}\frac{\partial}{\partial t}\left[-\frac{1}{c}\frac{\partial \bar{A}}{\partial t} - \text{grad } \phi\right]$$

Since $$\text{Curl Curl } \bar{A} = [\nabla \times \nabla \times A] = \bar{\nabla}\cdot\bar{\nabla}\bar{A} - \bar{\nabla}\bar{\nabla}\cdot\bar{A}$$

$$[\text{grad div } \bar{A} - \Delta \bar{A}] = \frac{4\pi\bar{J}}{c} - \frac{1}{c^2}\frac{\partial^2 A}{\partial t^2} - \frac{1}{c}\text{grad}\frac{\partial \phi}{\partial t}$$

$$\text{grad}\left[\text{div } \bar{A} + \frac{1}{c}\frac{\partial \phi}{\partial t}\right] = \frac{4\pi\bar{J}}{c} + \Delta\bar{A} - \frac{1}{c^2}\frac{\partial^2 A}{\partial t^2} \qquad 9.11$$

To reduce this so it will be true for Maxwell's equations we impose the so-called "normalization" of $\bar{A}$, or the Lorentz condition, that

$$\text{div } \bar{A} + \frac{1}{c}\frac{\partial \phi}{\partial t} = 0 \qquad 9.12$$

so (9.11) becomes

$$\Delta\bar{A} - \frac{1}{c^2}\frac{\partial^2 \bar{A}}{\partial t^2} = -\frac{4\pi\bar{J}}{c} \qquad 9.13$$

which reduces to the simple wave equation when $\bar{J}$ is zero.

Building another Hamiltonian

Our next discussion will be an attempt to describe the motion of charged particles in an electromagnetic field from the classical standpoint; i.e. building the Hamiltonian.

We use the same method as developed for the Schrödinger Hamiltonian where for the variational problem

$$I = \int L \, d\, t \quad \text{where} \quad L = T - V$$

and the momenta are defined by

$$p_i = \frac{\partial L}{\partial \dot{x}_i} \qquad 10.1$$

Solving these equations gives the Hamiltonian

$$H = T + V \qquad 10.2$$

At the beginning of this paper we mentioned the equations of motion for a charged particle in an electromagnetic field where the radiation reaction term was included. For the present we will make the assumption that this term is absent and then the pondermotive equation will be

$$\vec{F} = m\dot{\vec{V}} = e[\vec{E} + \vec{V}/c \times \vec{H}] \qquad 10.3$$

These equations are the Euler-Lagrange equations of the variational principle.

$$\delta \int L dt = 0$$

When $$\vec{H} = \text{Curl } \vec{A}$$

and $$\vec{E} = \frac{1}{c}\frac{\partial \vec{A}}{\partial t} - \text{grad } \phi$$

as shown in the preceeding section,

then $$L = M_e/2[\dot{X}^2 + \dot{Y}^2 + \dot{Z}^2] + e/c\ (\dot{X} A_x + \dot{Y} A_y + \dot{Z} A_z) - e\phi \qquad 10.4$$

The momenta which are canonically conjugate to the coordinates are given by

$$\begin{aligned} p_x &= \frac{\partial L}{\partial \dot{X}} = M_e\dot{X} + A_x\, e/c \\ p_y &= \frac{\partial L}{\partial \dot{Y}} = M_e\dot{Y} + A_y\, e/c \\ p_z &= \frac{\partial L}{\partial \dot{Z}} = M_e\dot{Z} + A_z\, e/c \end{aligned} \qquad 10.5$$

and from above

$$\begin{aligned} \dot{X} &= 1/M_e\ (p_x - e/c\ A_x) \\ \dot{Y} &= 1/M_e\ (p_y - e/c\ A_y) \\ \dot{Z} &= 1/M_e\ (p_z - e/c\ A_z \end{aligned} \qquad 10.6$$

Putting (10.4) and (10.5) into the Hamiltonian function then

$$H = \sum_i p_i\dot{X}_i - L = p_x\dot{X} + p_y\dot{Y} + p_z\dot{Z} - \frac{M_e}{2}[\dot{X}^2 + \dot{Y}^2 + \dot{Z}^2]$$
$$- e/c\ (\dot{X}A_x + \dot{Y}A_y + \dot{Z}A_z) + e\phi$$
$$H = (M_e\dot{X} + A_x\, e/c)\,\dot{X} + (M_e\dot{Y} + A_y\, e/c)\,\dot{Y} + (M_e\dot{Z} + A_z\, e/c)\,\dot{Z}$$
$$- \frac{M_e}{2}[\dot{X}^2 + \dot{Y}^2 + \dot{Z}^2] - e/c\ (\dot{X}A_x + \dot{Y}A_y + \dot{Z}A_z) + e\phi$$

Expanding and simplifying

$$H = M_e/2\ (\dot{X}^2 + \dot{Y}^2 + \dot{Z}^2) + e\phi$$

Putting in the values from (10.6)

$$H = \frac{1}{2M_e}\left[(p_x - e/c\ A_x)^2 + (p_y - e/c\ A_y)^2 + p_z - e/c\ A_z)^2\right] + e\phi \qquad 10.7$$

This is a classical Hamiltonian of a particle in an electromagnetic field

These equations may be carried over into the quantum theory by substituting into

$$H\psi = \frac{hi}{2\pi}\frac{\partial\psi}{\partial t} \qquad 10.8$$

(10.8) is the time dependent Schrödinger equation. If resolved to a vector equation then (10.7) is

$$H = \frac{1}{2M_e}\left[(\bar{p} - e/c\ \bar{A})^2 + e\phi\ \right] \qquad 10.9$$

This equation gives rise to infinities in the classical theory of the electron.

Eliezer's Work on Dirac's Elimination of Infinities

Dirac proposed that the infinities occurring in the Classical theory could be attributed to the fact that the electron was not considered an "elementary particle". The infinite self energy that shows up in the solution, which is the result of the work that has to be done against electromagnetic forces in concentrating the finite charge to a point, may be eliminated if we follow the above principle and state that the electron can not be further divided.

In his formulation of classical electrodynamics he assumed that the electromagnetic potentials be expressed as a four vector A_u which is made up of the vector and scalar potential of the previous section. The charge

current density vector j_u is made up of $\bar{J}$ and ρ. You may recall that for the Dirac electron in the electrostatic field we made the restricting assumption that only an electrostatic field was present. In reality this is impossible because a magnetic field which is absent, with respect to one observer, will be present with respect to another.

The coordinates of space and time at any point are X_i where i = 1,2,3,4 and the metric tensor, when the velocity of light is unity, is

$$g_{uv} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \qquad 11.1$$

He assumed that the world line of the electron in space-time is $Z_u = Z_u(S)$ where S is the proper time.

At the point X_u the above mentioned potentials satisfy the equations

$$\frac{\partial A_u}{\partial X_u} = 0 \quad \text{and} \quad \Box A_u = 4\pi j_u \qquad 11.2$$

where

$$\Box \equiv \frac{\partial^2}{\partial X_1^2} + \frac{\partial^2}{\partial X_2^2} + \frac{\partial^2}{\partial X_3^2} - \frac{\partial^2}{\partial X_4^2} \qquad 11.3$$

The next bold assumption that was made was the inclusion of advanced potentials to express the field of the electron. This is the point where Eliezer departed a little from Dirac's Theory. Dirac had considered that the field of the electron was just a retarded field.

$$F_{el} = F_{ret} \qquad 11.4$$

Since this is the basic assumption of the Maxwell-Lorentz theory it was not unusual that the same equation of motion resulted from both the Lorentz and Dirac theory.

Choosing a proper function G, Eliezer expressed the field of the electron as

$$F_{el} = F_{ret} + G = F_{ret} + k(F_{ret} - F_{adv}) \qquad 11.5$$

The total field, where k is an arbitrary constant, was represented by

$$F = F_{el} + F_{ext} \qquad 11.6$$

where F_{ext} is the external electromagnetic field.

A new field may be defined as

$$f = F - 1/2(F_{ret} + F_{adv}) \qquad 11.7$$

If (11.5) is inserted into (11.6), after which (11.6) is put into (11.7) then

$$f = F_{ret} + k(F_{ret} - F_{adv}) + F_{ext} - 1/2\ (F_{ret} + F_{adv})$$

and $$f = (k + 1/2)(F_{ret} - F_{adv}) + F_{ext} \qquad 11.8$$

If this is expressed on the world line then

$$f^{u\sigma} = 2/3(2k + 1)e(v^{\sigma} \frac{d^2v^u}{ds^2} - v^u \frac{d^2v^{\sigma}}{ds^2}) + F_{ext} \qquad 11.9$$

Eliezer developed the equations of motion in terms of this field by using the principles of conservation of energy, momentum and angular momentum. The resulting equation is

$$m \frac{dv_u}{ds} = ev_{\sigma} f_u^{\sigma} \qquad 11.10$$

If we insert (11.9) then

$$m \frac{dv_u}{ds} - 2/3\ e^2\ (2k + 1)[\ \frac{d^2v_u}{ds^2} + (\frac{dv}{ds})^2 v_u\ ] = ev_{\sigma} F_u^{\sigma}\ ext \qquad 11.11$$

where $$v^2 = v_u v^u = 1$$

Different choices of the arbitrary constant k will lead to three different types of equations. First if $2k + 1 > 0$ then equations will result

which are of the Dirac type, but the numerical value will be changed by a factor of $2k + 1$. This, however, results in non-physical solutions which are contrary to classical theory. Solution of the equations reveals that the electron instead of spiraling into the nucleus, will travel toward the nucleus acquiring a negative acceleration which increases until somewhere near the nucleus the electron changes its direction and escapes to infinity. When $2k + 1 < 0$ then the radiation field is just opposite to the first case. The third and last case is when $2k + 1 = 0$ and $k = -1/2$. This is found the most practical for solving problems with classical methods. Such a choice causes the elimination of the radiation reaction term which allows the existence of stationary states. The resulting equations for a single particle is

$$m \frac{dv_u}{ds} = ev_\sigma F_u^\sigma \text{ ext} \qquad 11.12$$

Eliezer pointed out that the absence of the radiation damping term in the case of the single electron possibly would be correct. The term should be applied only in the case of many particles where there are interactions between electrons.

The special theory of relativity may be applied to formulate (11.12). If radiation damping is included the general theory of relativity is necessary.

The entire basis of relativistic electrodynamics is the joining of the $\bar{H}$ and $\bar{E}$ vectors into one skewsymmetric world tensor of rank 2 to represent the field, namely $F_{u\nu}$. If the potentials ($\bar{A}$ and ϕ) are represented by the world vector potential A_u then the relationship between field and potentials is as follows.

$$F_{u\nu} = \frac{\partial A_u}{\partial X_u} - \frac{\partial A_\nu}{\partial X_u} \qquad 11.13$$

and

$$\frac{\partial F_{u\nu}}{\partial X_\lambda} + \frac{\partial F_{\nu\lambda}}{\partial X_u} + \frac{\partial F_{\lambda u}}{\partial X_\nu} = 0 \qquad 11.14$$

If the indices of the field are raised then the following relationship exists:

$$\frac{\partial F^{u\nu}}{\partial X_\nu} = 4\pi j^u \qquad 11.15$$

where j^u is made up of $\bar{J}$ and ρ.

Using the relationship $\frac{\partial A_u}{\partial X_u} = 0$ and inserting (11.13) with raised indices into (11.15)

$$\frac{\partial}{\partial X_\nu}\left(\frac{\partial A^u}{\partial X_\nu}\right) - \frac{\partial}{\partial X_\nu}\left(\frac{\partial A^\nu}{\partial X_u}\right) = 4\pi j^u$$

$$\therefore \frac{\partial^2 A^u}{\partial X^2_\nu} = 4\pi j^u$$

If we form the divergence of (11.15), that is

$$\frac{\partial}{\partial X_u}\frac{\partial F^{u\nu}}{\partial X_\nu} = 4\pi \frac{\partial j^u}{\partial X_u}$$

then

$$\frac{\partial j^u}{\partial X_u} = 0 \qquad 11.16$$

Equations (11.13), (11.14), (11.15) and (11.16) are new forms of Maxwell's Equations. Using these equations as a basis then we may write down the relativistic Lagrangian which is similar to the non-relativisitc one (10.4).

Here we will accept the Minkowski world where s is considered the proper time. It may be expressed in terms of the space and time coordinates as follows

$$ds = (dX_4^2 - dX_1^2 - dX_2^2 - dX_3^2)^{1/2} \qquad 11.17$$

or in terms of the metric tensor $g_{u\nu}$ as

$$ds = (g_{u\nu}\, dX^u\, dX^\nu)^{1/2} \qquad 11.18$$

Therefore with s as parameter the Lagrangian is

$$L(s) = -1/2\, M_e g_{u\nu} \frac{dX^u}{ds} \frac{dX^\nu}{ds} + e\frac{dX^u}{ds} A_u$$

or since

$$\frac{dX^u}{ds} = v^u$$

then

$$L(s) = -1/2\, M_e g_{u\nu}\, v^u v^\nu + e v^u A_u \qquad 11.19$$

If we lower the index by

$$v_u = g_{u\nu}\, v^\nu \quad \text{and} \quad v_u v^u = v^2$$

then (11.19) is

$$L(s) = -1/2\, M_e v^2 + e v^u A_u$$

The momenta may be expressed by

$$p_\sigma = \frac{\partial L}{\partial v^\sigma} = -M_e v_\sigma + e\frac{\partial v^\sigma}{\partial v^\sigma} A_\sigma$$

so

$$p_\sigma = -M_e v_\sigma + eA_\sigma \qquad 11.20$$

If the equations of motion are expressed in terms of the Euler-Lagrange equations of motion

$$\frac{d}{ds}\left(\frac{\partial L}{\partial v^\sigma}\right) - \frac{\partial L}{\partial X^\sigma} = 0$$

we have

$$\frac{d}{ds}\left(-M_e v_\sigma + eA_\sigma\right) - \frac{\partial}{\partial X^\sigma}\left(e v^u A_u\right) = 0$$

$$-M_e \frac{dv_\sigma}{ds} + e\frac{dA_\sigma}{ds}\frac{\partial X^u}{\partial X^u} - e v^u \frac{\partial A_u}{\partial X^\sigma} = 0$$

since

$$\frac{\partial X^u}{\partial s} = v^u$$

then

$$- M_e \frac{dv_\sigma}{ds} + e v^u \frac{dA_\sigma}{dX^u} - e v^u \frac{\partial A_u}{\partial X^\sigma} = 0 \qquad 11.21$$

If we use (11.13) where $F_{uv} = \frac{\partial A_u}{\partial X_v} = \frac{\partial A_v}{\partial X_u}$

then (11.21) becomes

$$- M_e \frac{dv_\sigma}{ds} = e v^u F_{\sigma u}$$

and

$$M_e \frac{dv_\sigma}{ds} = e v_u F_\sigma{}^u \text{ ext} \qquad 11.22$$

is the same equation that was derived by Eliezer from the

$$k = - 1/2$$

The three spatial equations which are more familiar and come directly from (11.22) are

$$\frac{d}{dt} \frac{M_e \bar{V}}{\sqrt{1 - V^2}} = e[\bar{E} + (\bar{V} \times \bar{H})]$$

Building a Hamiltonian for the electron in the Electromagnetis Field

We have found in the last section that to solve problems under the classical theory, it is necessary to make certain restrictions in order that good solutions will result. However, to take the classical equations over into the Quantum theory we can make the assumption that it would be immaterial which form of the classical equations be used for we would find consistent results from the Quantum equation.

Certain discontinuties which arise when the equation of motionare transferred to the Hamiltonian theory, may be eliminated by using a process introduced by Wentzel and developed by Dirac. This process, called the

λ- Limiting process uses the principle of a small time like vector λ_u taken so that $\lambda^2 > 0$ and $\lambda_4 > 0$ 12.1

If the potential satisfies the equation

$$\Box A_u = 0 \qquad 12.2$$

the Poisson bracket using this potential in terms of the λ is

$$[A_u(X), A_\sigma(X)] = 1/2\, g_{u\sigma} [\Delta(X - X' + \lambda) + \Delta(X - X' - \lambda)] \qquad 12.3$$

where use has been made of the Jordan-Pauli Δ function.

The momentum which is found for such potentials is of the same form (11.20) found in the discussion of the special theory of relativity, namely

$$p^u = M_e v^u + eA^u \qquad 12.4$$

We found in Section (2) that the general formula for the Hamiltonian was

$$H = - L + p\dot{X} \qquad 12.5$$

The Lagrangian is found from (12.4) by

$$p^u = \frac{\partial L}{\partial v^u}$$

or
$$L = \frac{M_e v^2}{2} + eA^u v^u \qquad 12.6$$

from (12.5)
$$\dot{X}^u = v^u - \frac{p^u - eA^u}{M_e} \qquad 12.7$$

If (12.6) and (12.7) are put in (12.5)

$$H = - \frac{M_e}{2} \left(\frac{p^u - eA^u}{M_e}\right)^2 + eA^u v^u + p^u \left(\frac{p^u - eA^u}{M_e}\right)$$

$$H = - \frac{1}{2M_e} (p^u - eA^u)^2 - eA^u v^u + \frac{p^2}{M_e} - \frac{p^u eA^u}{M_e}$$

$$H = - \frac{1}{2M_e} (p^u - eA^u)^2 - eA^u v^u + \frac{M_e^2 v^2}{M_e} - \frac{eA^u v^u M_e}{M_e}$$

and as in the original classical theory $v^2 = 1$

So $$H = - \frac{1}{2M_e} (p^u - eA^u)^2 + M_e$$

or $$H = - \frac{1}{2M_e} [(p^u - eA^u)^2 - M_e] \qquad 12.8$$

Elimination of Divergences in the Solution of the Hydrogen Atom in a Radiation Field

It is known that the theory of Pauli and Heisenberg, especially when applied to the photon theory, allowed only positive energy states. This restriction eliminated some of the difficulties; however, it introduced infinities into the solutions of the wave equations. Dirac showed that for even values of n the integrals resulting when the λ limiting process is used, namely

$$\int_o^\infty f(k_4) \cos \lambda_4 \; k_4 \, dk_4$$

are without divergence but for odd n the divergence reappears. He assumed that both positive and negative energy states should be represented so the integral became

$$1/2 \int_{-\infty}^{\infty} \{ f(k_4) \; e^{ik_4\lambda_4} + f(-k_4) \; e^{-k_4\lambda_4} \} \, dk_4 \qquad 13.1$$

The divergences encountered in the radiation theory are eliminated by the use of this integral. The wave functions are expressed in terms of negative energy photons and also positive energy photons, namely ξ_- and ξ_+

Probability of state with $m + n$ photons where m is the positive number and n the negative are found from the coefficients of $\xi_+^m \; \xi_-^n$
If we consider this as m photons emitted and n photons absorbed then the conservation principles are satisfied in regard to negative energy.

For the problem of the Hydrogen atom we use the Hamiltonian found in

(12.8) and carry it to the quantum theory by the equation.

$$[(p^u - eA^u)^2 - M_e]\Psi = 0 \qquad 13.2$$

We find that this equation does not include the spin of the electron so it must be transformed to

$$[p_4 - eA_4 - \bar{\alpha}.(\bar{p} - e\bar{A}) - M_e\beta]\Psi = 0 \qquad 13.3$$

where $\bar{\alpha}$ and β are the usual Dirac matrices that were given in earlier theory and

$$p_4 = i\frac{\partial}{\partial x_4} \quad ; \quad \bar{p} = -i\frac{\partial}{\partial \bar{x}}$$

The velocity of light and $h/2\pi$ are considered unity.

A_4 which is the potential due to the nucleus may be represented by $-Ze/r$. Therefore the equation becomes

$$[p_4 + Ze^2/r - \bar{\alpha}.(\bar{p} - e\bar{A}) - M_e\beta]\Psi = 0 \qquad 13.4$$

We turn to the time dependent perturbation theory for the solution. The Ψ function is expanded in a power series of the charge

$$\therefore \Psi = \Psi_0 + e\Psi_1 + e^2\Psi_2 + \ldots \qquad 13.5$$

If this is substituted in (13.4) which is of form $H\Psi = i\partial\Psi/\partial x_4$ then

$$(p_4 + Ze^2/r - \bar{\alpha}.(\bar{p} - e\bar{A}) - M_e\beta)[\Psi_0 + e\Psi_1 + e^2\Psi_2 + \ldots] = 0$$

$$\therefore p_4\Psi_0 + Ze^2/r\,\Psi_0 - \bar{\alpha}.p\Psi_0 + e\bar{\alpha}.\bar{A}\Psi_0 - M_e\beta\Psi_0$$
$$+ e\,Ze^2/r\,\Psi_1 - e\Psi_1\bar{\alpha}.\bar{p} + e^2\bar{\alpha}.\bar{A}\Psi_1 + ep_4\Psi_1 - eM_e\beta\Psi_1$$
$$+ e^2p_4\Psi_2 + e^2\,Ze^2/r\,\Psi_2 - e^2\Psi_2\bar{\alpha}.\bar{p} - e^3\Psi_2\bar{A}$$
$$- e^2M_e\beta\Psi_2 + \ldots = 0$$

Equating coefficient of e

$$[p_4 + Ze^2/r - \bar{\alpha}.\bar{p} - M_e\beta]\Psi_0 = 0 \qquad 13.6$$

$$[p_4 + Ze^2/r - \bar{\alpha}.\bar{p} - M_e\beta]\Psi_1 = -\bar{\alpha}.\bar{A}\Psi_0 \qquad 13.7$$

$$[p_4 + Ze^2/r - \bar{\alpha}.\bar{p} - M_e\beta]\Psi_2 = -\bar{\alpha}.\bar{A}\Psi_1 \qquad 13.8$$

(13.6) is nothing more than the time dependent equation which is analagous to the time independent equation that was solved in section (8). If we assume that there are no photons present and take the atom in the stationary state then we may substitute into (13.6)

$$\Psi_o = \psi_n^o e^{-i E_n X_4} \qquad 12.9$$

where ψ_n^o are the eigenfunctions of Section (8) and E_n is the E of (8.26)

That is $E_n = M_e n_n^{1} [n_n^{1^2} + e^4]^{-1/2}$

n_n^{1} being equivalent to n^{1} only it is expressed in terms of $h/2\pi$ and c being unity.

Equation (13.7) may be expressed as

$$[p_4 + Ze^2/r - \bar{\alpha}.\bar{p} - M_e \beta]\Psi_1 = -\bar{\alpha}.\bar{A}\psi_{ne}^{o} e^{-i M_e n_n^{1} [n_n^{1^2} + e^4]^{-1/2} X 4}$$

Solving, Eliezer found that Ψ_1 was expressed in terms of integrals

$$\int^{\infty} [(a - k_4)^{-1} - i\pi\delta(a - k_4)] k_4 e^{-ib k_4} dk_4$$

where a and b are independent of k_4 and the integral has the value zero. Because of this, Ψ_2 is zero and the remaining equations of higher order will automatically be zero.

Therefore, $\Psi_{nm} = 0$ for $m \neq n$; and all solutionswill be good solutions for the Hydrogen atom in the Electromagnetic Field.

Conclusions

We have started with the more elementary concepts, namely the non-relativistic Schrödinger equation which we find is just a special case of the relativistic Dirac equation of the electrostatic field. Examination of the Dirac equation for the electromagnetic field shows that his equation in the electrostatic field is just a special case of it. Therefore, the basic equation from which all others come is the Dirac Equation for the Electromagnetic field. Dirac's equations give us results which are in agreement with experiment; therefore, we must be sure that the postulates of Quantum Mechanics are everywhere satisfied and that the solutions to the equations are always finite.

After eliminating certain infinities in the classical equations we show by a λ limiting process and by a good interpretation of results that we are able to build equations that are finite for the problem of the hydrogen-like atom even in the higher orders.

We find, however, a very serious flaw in the above approach when the techniques are applied to the overall picture of particle theory. The common phenomena of generation and annilhilation of pairs of particles with opposite electric charges would be impossible from this standpoint. This is because of the condition under the λ limiting process where two particles may not be nearer than a distance λ ; an obvious impossibility for these phenomena.

It would appear that a new method of attack must be devised if we are to generate a theory that is consistent and finite in all cases.

Abstract

After a brief discussion about Lorentz's attempts to formulate a successful theory of particles using Maxwell's equations, we focus our attention on solutions of particle problems by quantum methods.

The problem of the electrostatic field is solved first. After building a Hamiltonian for the Hydrogen atom using the non-relativistic approach we carry our equations over into the quantum theory obtaining as a result the Schrödinger wave equation. Separation of this equation is carried out by letting the eigenfunction ψ be expressed in terms of three functions, namely $\psi = \Theta \Phi R$. For a solution of the Hydrogen atom we solve the R equation, that is split from the ψ, by a power series method. Infinities are eliminated and a Recursion Formula obtained. The Eigenvalues which represent the stationary states are found to be in agreement with the energy values of Bohr's orbits.

The eigenfunction for the ground state is examined and found to yield, when multiplied by its complex conjugate and integrated over all space, a charge distribution of a sphere for the hydrogen atom.

The next phase that is discussed is the effect of a time independent perturbation upon the Hydrogen Atom. After building a first and second order Rayleigh-Schrödinger Perturbation theory, it is applied to the case of a static electric field on the hydrogen atom and the polarization and the shift of spectral lines is observed.

The necessity for an explanation of the hyper fine struc ture in spectral lines led us to the Dirac Equation for an electron in an electrostatic field. Dirac's method is used to Linearize the quadratic H and then

this relativistic equation is carried over to the Quantum theory. The solution is carried through with the help of matrices where the ψ function was represented as a one by four matrix.

After incorporating the spin of the electron into the equations by use of the Dirac matrices α_X, α_Y, α_Z and α_m the two radial equations were separated from the equations by use of the constants of motion. These two equations are solved by means of power series and from the Recursion formula we are able to get Energy Eigenvalues which differ from the Bohr values by an amount equal to the added affects. Subtraction of the rest energy $M_e c^2$ from the eigenvalues gives us the Sommerfeld fine structure formula. Here both negative and positive states of energy are allowed where under the Schrödinger theory only positive states exist. Quantized values of Energy range between $-M_e c^2$ and $+M_e c^2$ and continuous spectrum of values extends from each.

A shift to the electromagnetic field shows that two potentials are present, one a vector and the other a scalar represented as $\bar{A}$ and ϕ respectively.

These potentials are specified in terms of Maxwell's equations after which the continuity and wave equations are derived. The latter is accomplished by a Normalization of $\bar{A}$, better known as the Lorentz condition.

A non-relativistic Hamiltonian is formed in terms of the potentials. The classical equations of motion are found to produce infinities which we are able to remove by using Eliezer's process. The resulting equations are examined for the different solutions obtained from the choice of an arbitrary constant k. A choice of k such that the radiation reaction term

was eliminated was found the best for it allowed the existence of stationary states in the Classical theory.

Equations derived from the special theory of relativity are found to agree with the equations when the radiation reaction term is zero; which indicated that Eliezer's equations are consistent with the special theory of relativity.

Now that we have a finite classical equation, it must be carried over to the Quantum theory. This was accomplished most successfully by Dirac when by use of a λ limiting process where η is a time like vector, he built a Hamiltonian for an electron in an electromagnetic field. By the λ process, it is impossible for two particles to come closer than a distance λ.

A time dependent perturbation process is used to solve the equation of the Hydrogen Atom by which we are able to obtain convergent values for the wave functions. In the conclusions we find that all of the equations discussed are modifications of the Dirac equation for the electron in the electromagnetic field.

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